MICROWAVE SPECTROSCOPY OF 2-METHOXYETHYLAMINE-WATER: STRUCTURAL CHANGES DUE TO HYDROGEN BONDING NETWORKS

NATHAN HARPER[a], *Department of Chemistry, Emory University, Atlanta, GA, USA*; BRITTANY BASENBACK, RANIL GURUSINGHE, MICHAEL TUBERGEN, *Department of Chemistry and Biochemistry, Kent State University, Kent, OH, USA*.

2-Methoxyethylamine (2MEA) exists in trans and gauche conformations, each with at least one intramolecular hydrogen bond from the amine to the methoxy oxygen. Rotational spectra of 2MEA, recorded by Caminati et al., exhibit splittings arising from methyl internal rotation tunneling (V_3 = 822.6 cm^{-1} and 1102cm^{-1} respectively).[b, c] We report the rotational spectra of the three ^{13}C isotopologues for each 2MEA conformer. The rotational transitions, including resolved tunneling splittings and nuclear quadrupole hyperfine components, were fit with XIAM.[d] Ab initio calculations (MP2/6-311++G(d,p)) were used to model stable structures of 2MEA-water complexes. The most stable structure of the 2MEA-water complex was found to have an intermolecular hydrogen bond from the water to the amine and an intramolecular hydrogen bond from the amine to the methoxy oxygen. Twenty-five rotational transitions of 2MEA-water were recorded (A = 2922.74(3) MHz, B = 1696.72(2) MHz, and C = 1379.80(2) MHz) and assigned to the lowest-energy structure of the complex. Methyl internal rotation tunneling splittings were not resolved in the spectrum of 2MEA-water. The formation of hydrogen bonding networks in the 2MEA-water complex was found to alter the configuration of 2MEA within the complex.

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[a] Summer 2017 REU student at Kent State University

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[d] H. Hartwig and H. Dreizler, *Z. Naturforsch, A: Phys. Sci.* **51**, 923-932 (1996).